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Comparing SeaWiFS Reprocessing Versions (R3 vs. R4)

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ABSTRACT

Satellite observations of global ocean chlorophyll from SeaWiFS were recently reprocessed to incorporate calibration and algorithm improvements. Here, comparisons are made between the newly reprocessed SeaWiFS Level-3 chlorophyll product and the previous version using in situ measurements. The results show that the newly reprocessed SeaWiFS data matches up better with the surface measurements than the previous version did. Globally, the slope of the match-ups improves to 0.85 from 0.78 in log-log scale. A significant trend that contributed to this improvement was the overall decrease in SeaWiFS chlorophyll levels less than 1.0 mg m^{-3}. Regional analyses reveal that the match-ups improve in every oceanic basin, except the Antarctic. However, SeaWiFS continues to exhibit poor correspondence with in situ data in the North Atlantic where the match-ups have a slope of 0.54. Also, an examination of monthly images for May 1999 revealed that the number and magnitude of high-value chlorophyll pixels had increased in the high-latitude open ocean of the South Pacific.

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1. INTRODUCTION

Obtaining accurate measurements of chlorophyll concentration in the world's oceans is critical to our understanding of many biogeochemical processes. Chlorophyll is the green photosynthetic pigment in microscopic plants called pyhtoplankton. Through photosynthesis, phytoplankton play an important role in the Earth's carbon cycle and may mitigate global warming by transferring heat-absorbing carbon dioxide from the atmosphere back into the biosphere.

Satellite observations from the Sea-viewing Wide Field-of-view Sensor (SeaWiFS) have provided a continuous record of global ocean chlorophyll since September 1997. The near-global coverage and continuity of the SeaWiFS record permit observations of the spatial variability of phytoplankton through time, especially on seasonal and interannual timescales, and therefore, has vastly improved the capacity for modeling primary productivity and the carbon cycle.

Recently, SeaWiFS data was reprocessed to incorporate calibration and algorithm improvements. This study examines the newly reprocessed SeaWiFS product by comparing it to the previous version and utilizing in situ measurements to highlight differences.

2. DATA / METHODS

SeaWiFS daily and monthly chlorophyll data were obtained from the NASA Goddard Earth Sciences (GES)/Distributed Active Archive Center (DAAC). The data used for these analyses were Level-3 global 'Standard Mapped Images' (SMI) of mean chlorophyll-*a* concentration at approximately 9-km resolution from September 1997 through May 2002.

The SeaWiFS project recently reviewed instrument calibration, algorithms, and the operational procedures used to process the data [details are described in a forthcoming NASA Technical Memorandum by the SeaWiFS Project (Patt et al., in press) and on their Web site: http://seawifs.gsfc.nasa.gov/SEAWIFS/RECAL/Repro4/]. As a result, a complete mission reprocessing (September 1997 through present) was undertaken and the new data set (SeaWiFS Reprocessing #4 [R4]) was made available to the public in August 2002. The previous round of processing (SeaWiFS Reprocessing #3 [R3]) was completed in May 2000 and remained operational until July 2002.

To assess the changes made to the SeaWiFS globally mapped chlorophyll product in the newly reprocessed version (R4) from the previous operational data set (R3), a series of quantitative and qualitative comparisons were made. Both the new reprocessing (R4) and the last reprocessing (R3) of SMI data were used in conjunction with in situ data to obtain an independent comparison between the two different reprocessings.

2.1 SeaBASS Comparison

The in situ chlorophyll measurements were obtained from the SeaBASS (SeaWiFS Bio-Optical Archive and Storage System) data set (Werdell and Bailey, 2002). Over 32,000 measurements of fluorometrically/spectrophotometrically-derived chlorophyll-*a* (mg m^{-3}) at depths of 0.0 to 10.0 meters were available for the SeaWiFS mission period of September 15, 1997, through June 1, 2002.

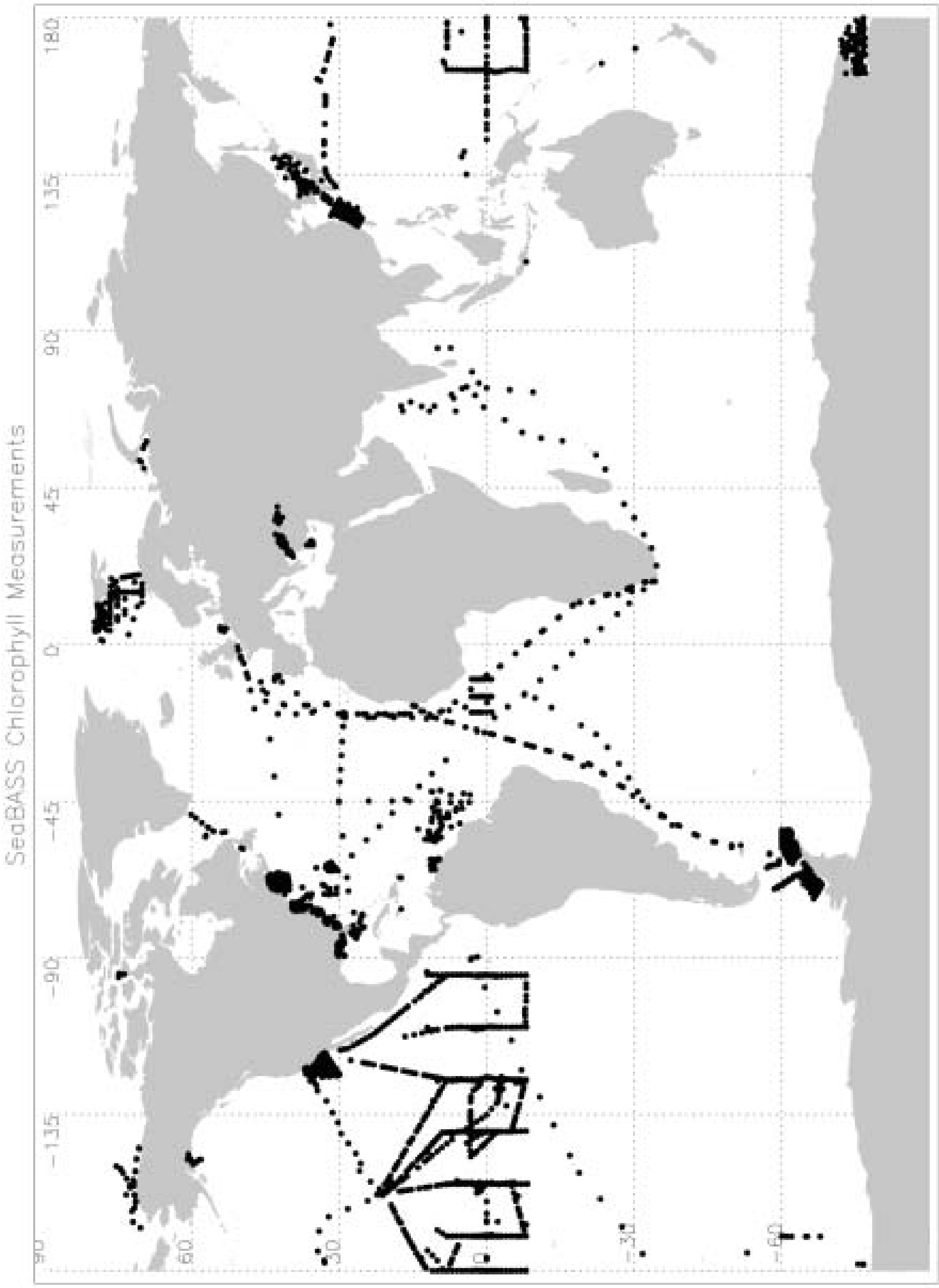


Figure 1. Global distribution of the in situ chlorophyll measurements taken at depths of 10.0 m or less (N= 32,587) from the SeaBASS archive for September 15, 1997, through June 1, 2002, as of June 4, 2002.

The available SeaBASS data for this time period were distributed through most of the world's major ocean basins (figure 1); however, many of the SeaBASS chlorophyll measurements were taken so close together in time that they should be considered duplicates in a daily pixel-level comparison. For example, within an 18-hour period on November 17, 1997, there were 13 surface-level chlorophyll measurements taken at the same latitude/longitude with similar readings (ranging from 1.03 to 1.89 mg m^{-3}). To compare each of these individual measurements with the same daily pixel value would unduly weight the results for this day. Therefore, a series of steps was taken to eliminate and/or average the in situ measurements taken at the same geographical position on the same day (at different times and/or different depths). First, the data were separated into records each with a unique day and latitude/longitude position, and the measurements within each record were sorted by depth. Measurements at the highest depths were assumed to best represent the surface chlorophyll concentration. One chlorophyll measurement was kept for each record by using the value obtained at the highest depth, or if there were multiple measurements taken at the highest depth (at different times on the same day), then these were averaged. This consolidated data set contained 20,483 values each corresponding to a unique day/latitude/longitude/depth. Therefore, the original extensive geographic distribution was preserved while avoiding the biasing problem of comparing the same SeaWiFS value to more than one in situ measurement for some days and not others.

Next, using the daily mapped SeaWiFS images (SMI) of chlorophyll-*a* concentration, the pixel corresponding to the date and location of the in situ value was identified. It should be noted that the pixel value obtained was considered to be representative of the day's concentration and thus this analysis does not take into account the time of day for in situ measurements or the overpass times of the satellite.

Due to missing data in the SeaWiFS SMI images, the number of SeaBASS measurements that matched up with SeaWiFS was 7,384 for R4 and 6,674 for R3. The new reprocessing algorithms increased the number of valid chlorophyll measurements and the spatial coverage of R4 expanded over that of R3. To directly compare the two reprocessed versions, however, only the 6,498 points where both R3 and R4 have a SeaBASS match-up were used. At this point, it was determined that additional data consolidation was necessary because in some cases, a great number of values from the adapted SeaBASS data set were being compared with the same 9-km pixel. For example, in one day (June 5, 1998) there were 30 measurements with a (slightly) unique latitude/longitude position, but each fell within the same SeaWiFS pixel. Comparing numerous point measurements with a single coarse resolution pixel value would skew the statistics. Therefore, the in situ values within one pixel were averaged for comparison with the SeaWiFS observations and at the same time, measurements with depths of greater than 5 meters were eliminated. This resulted in 2,470 SeaWiFS/SeaBASS match-ups (116 of which have identical values for R3 and R4). Figure 2 illustrates the geographical distribution of SeaBASS points that have a coincident SeaWiFS pixel for both data sets.

Statistical comparisons between the SeaWiFS data sets and the consolidated SeaBASS values were made. A land/ocean/coastal mask was created using topographic data (ETOPO5) consisting of land elevation and ocean depths. This data was at a slightly higher resolution (4320 x 2160) than the SeaWiFS mapped images and so was regridded to approximately 9-km resolution (4096 x 2048). Using this mask, statistics were generated for the global oceans as well for coastal (<= 200 m depth) and open ocean (> 200 m depth) areas. Root mean squared differences (RMSDs) and biases, as well as linear regression coefficients, were calculated for 13 major oceanic basins (shown in figure 2) in the native chlorophyll units and base 10 log scale. All of the comparative statistics reported herein are in log-log scale except for the medians.

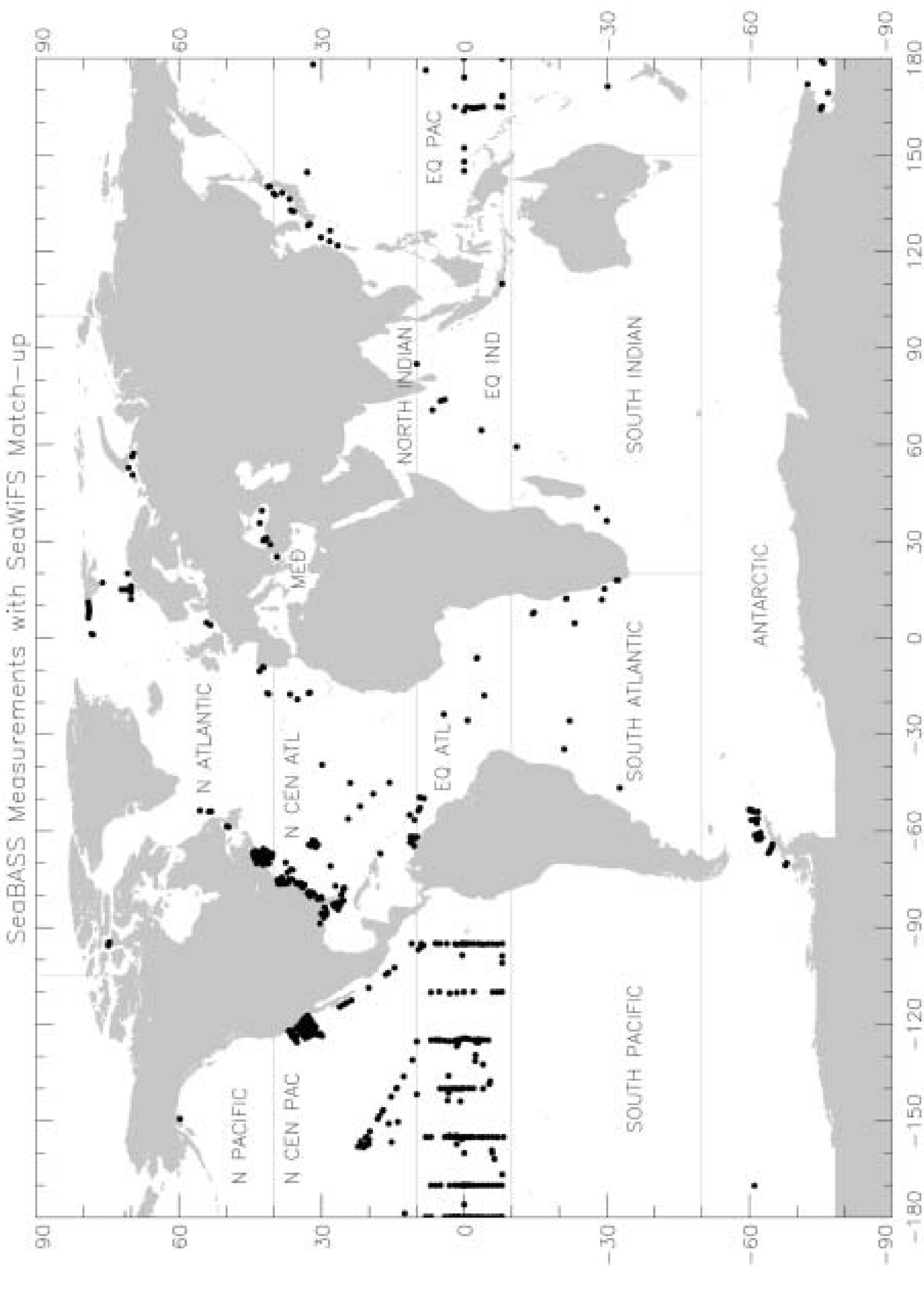


Figure 2. Global distribution of the SeaBASS measurements with a co-located SeaWiFS pixel for both R3 and R4 (N=2,470). The oceanic regions used for statistical comparisons are shown.

2.2 Monthly Comparison of SeaWiFS Reprocessings

A visual inspection of monthly SeaWiFS images revealed that R4 contained a noticeable increase in high chlorophyll pixels in some open ocean areas. Therefore, comparisons of R3 and R4 images (independent of the SeaBASS match-ups) were done to characterize the presence and magnitude of high outliers in high-latitude open ocean areas typically characterized by low chlorophyll. Mapped monthly data (9-km SMI) from May 1999 were chosen for this analysis because the SeaWiFS Project used these data in their reprocessing analyses.

3. RESULTS / DISCUSSION

3.1 Comparison of SeaWiFS Reprocessings using SeaBASS Match-Ups

The relationships between SeaWiFS R3/R4 and the SeaBASS match-up points are shown in figure 3. The global R4 match-ups are better aligned to the 1-to-1 line than the corresponding R3 values. This is reflected in the regression coefficients as well, with the R4 slope (at 0.85) significantly closer to 1.0 (in comparison, R3's slope was 0.78). However, the global r^2 values were similar at 0.78 for R4 and 0.77 for R3, and the scatter and bias were only slightly improved in R4 (R4 RMSD=0.29 and bias=0.06 versus R3 RMSD=0.28 and bias=0.09).

When directly comparing the R3 and R4 SeaWiFS measurements that have SeaBASS match-ups, it generally appears that the low chlorophyll values are lower for R4 as compared to R3 and vice-versa for high-chlorophyll areas (figure 4). This is also reflected in the regression coefficients (the slope is slightly greater than 1.0 and the y-intercept is less than 0.0). Taken as a whole, the number of points where R3 is greater than its R4 counterpart is almost 2 to 1. However, in low-chlorophyll areas where both R3 and R4 are < 1.0 mg m^{-3}, over 93% (1,009 values) have a higher R3 value than R4. Conversely, where both R3 and R4 are greater than 1.0 mg m^{-3}, the R4 values are greater than R3 in about 62% of the match-ups. While the difference between R3 and R4 in the high-chlorophyll match-ups may be significant, the most obvious trend is that R4 is almost always lower than R3 in match-ups with low chlorophyll values.

As stated before, the total number of valid pixels increased with the R4 version. Therefore, to determine whether any bias was present in the new R4 pixels, the 445 points where only R4 had a valid chlorophyll value (and R3 did not) were compared to the SeaBASS measurements (figure 5). The scatter is fairly high but the regression coefficients show that the majority (65%) of R4 values are greater than the corresponding in situ values. This comparison shows no evidence of bias in the newly added R4 values.

Regional match-ups between the two SeaWiFS data sets and SeaBASS show that there are some differences depending on the oceanic basin being compared. Twelve of the 13 regions shown in figure 2 have coincident points, but five regions have the most significant (> 40) number of match-up points: North Atlantic, North Central Atlantic, North Central Pacific, Equatorial Pacific, and Antarctic. The North Atlantic has the highest number of comparison points by far (N=1,323) so the global results are heavily impacted by this region. Figure 6 shows the comparison between SeaBASS and SeaWiFS R3/R4 for these five regions as well as the Mediterranean.

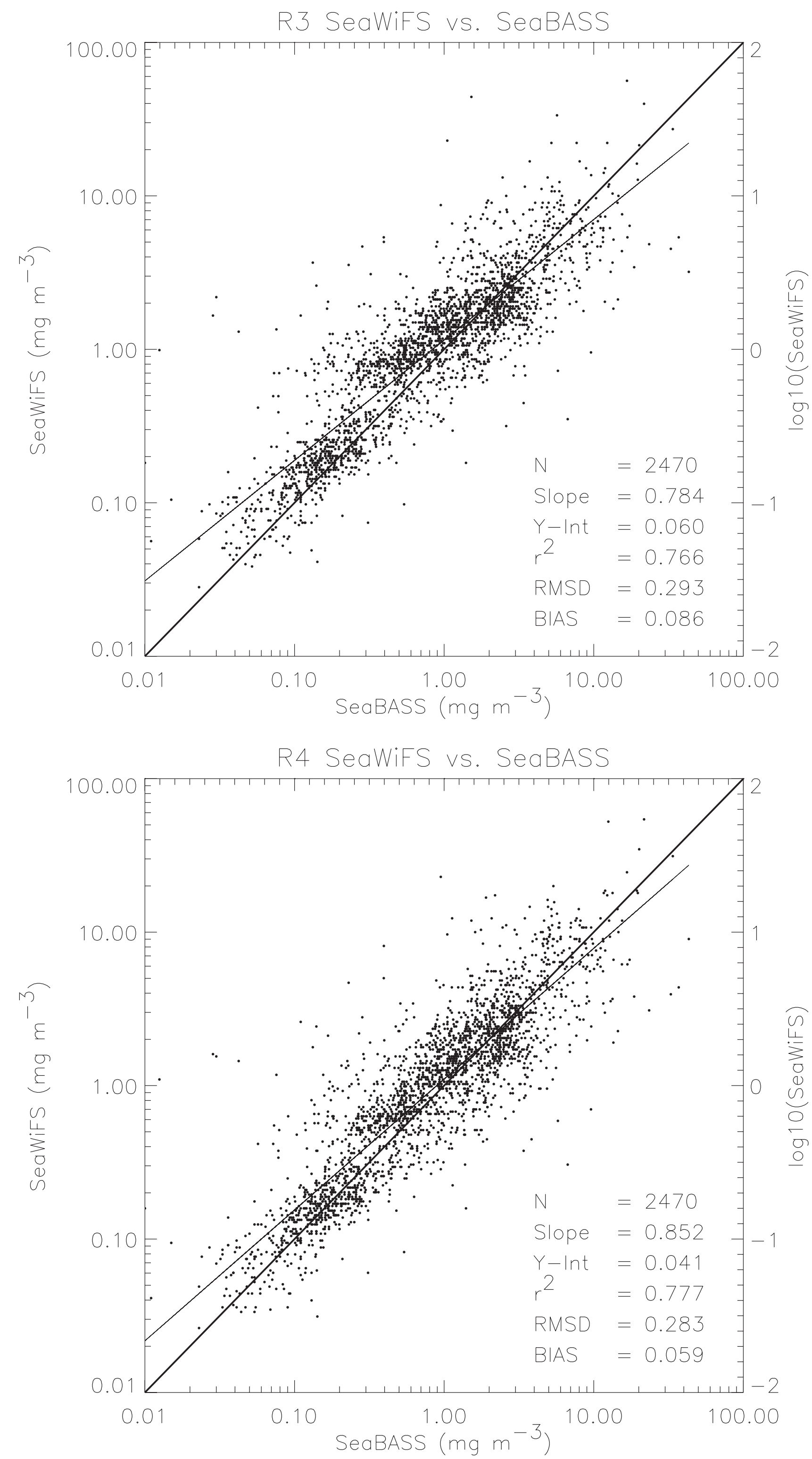


Figure 3. Scatterplots comparing SeaBASS chlorophyll measurements (mg m^{-3}) with co-located SeaWiFS values for versions R3 (top) and R4 (bottom). The 1-to-1 line (thick) and the least-squares regression line (thin) are shown, as well as regression coefficients, root mean squared differences (RMSDs), and biases.

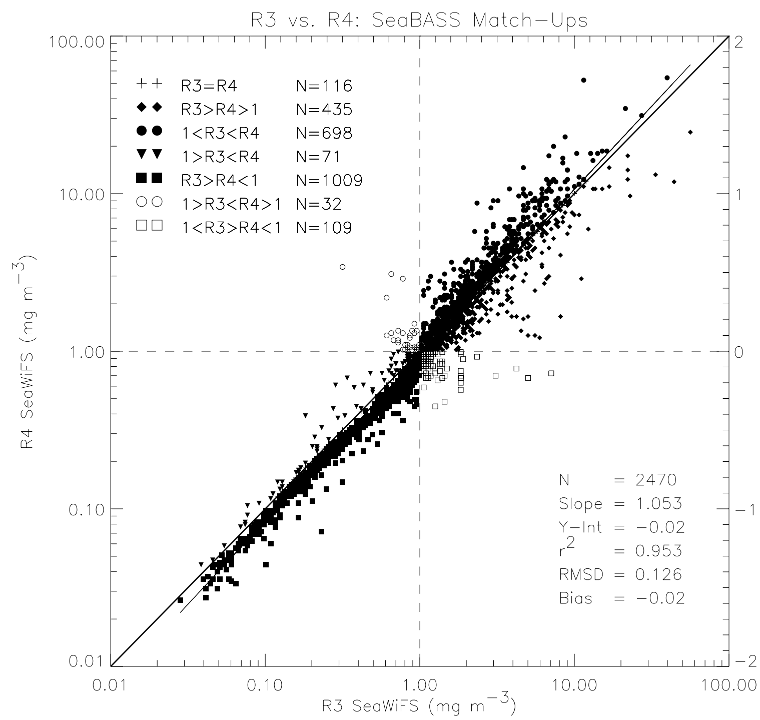


Figure 4. Scatterplot of SeaWiFS pixels with SeaBASS match-ups (R3 SeaWiFS versus R4 SeaWiFS). The 1-to-1 line (thick) and the least-squares regression line (thin) are shown, as well as the regression coefficients, RMSD and bias. The symbol representations are shown and the number of match-ups fitting each criteria are listed.

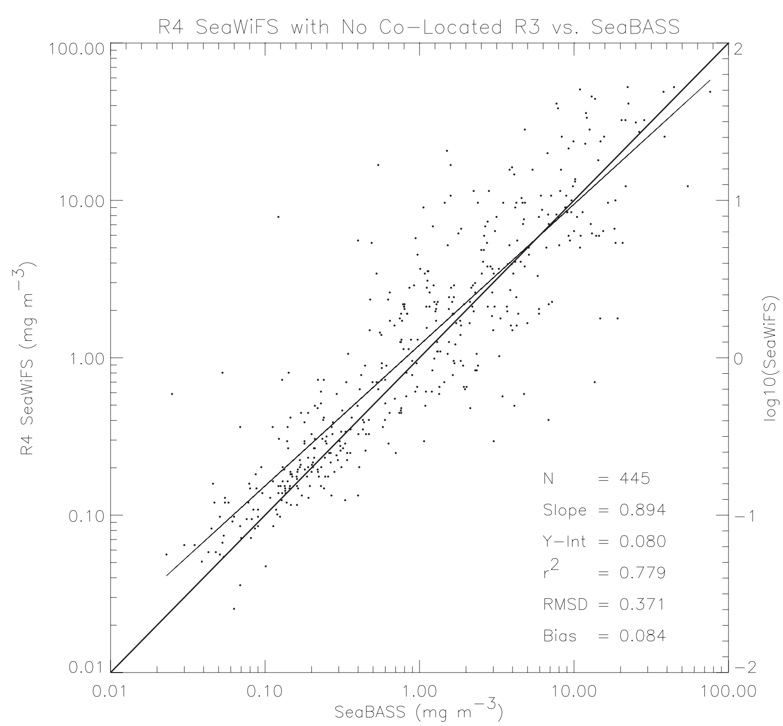


Figure 5. Scatterplot of R4 SeaWiFS pixels that did not have a valid coincident R3 pixel versus SeaBASS. The 1-to-1 line (thick) and the least-squares regression line (thin) are shown, as well as regression coefficients, RMSD and bias.

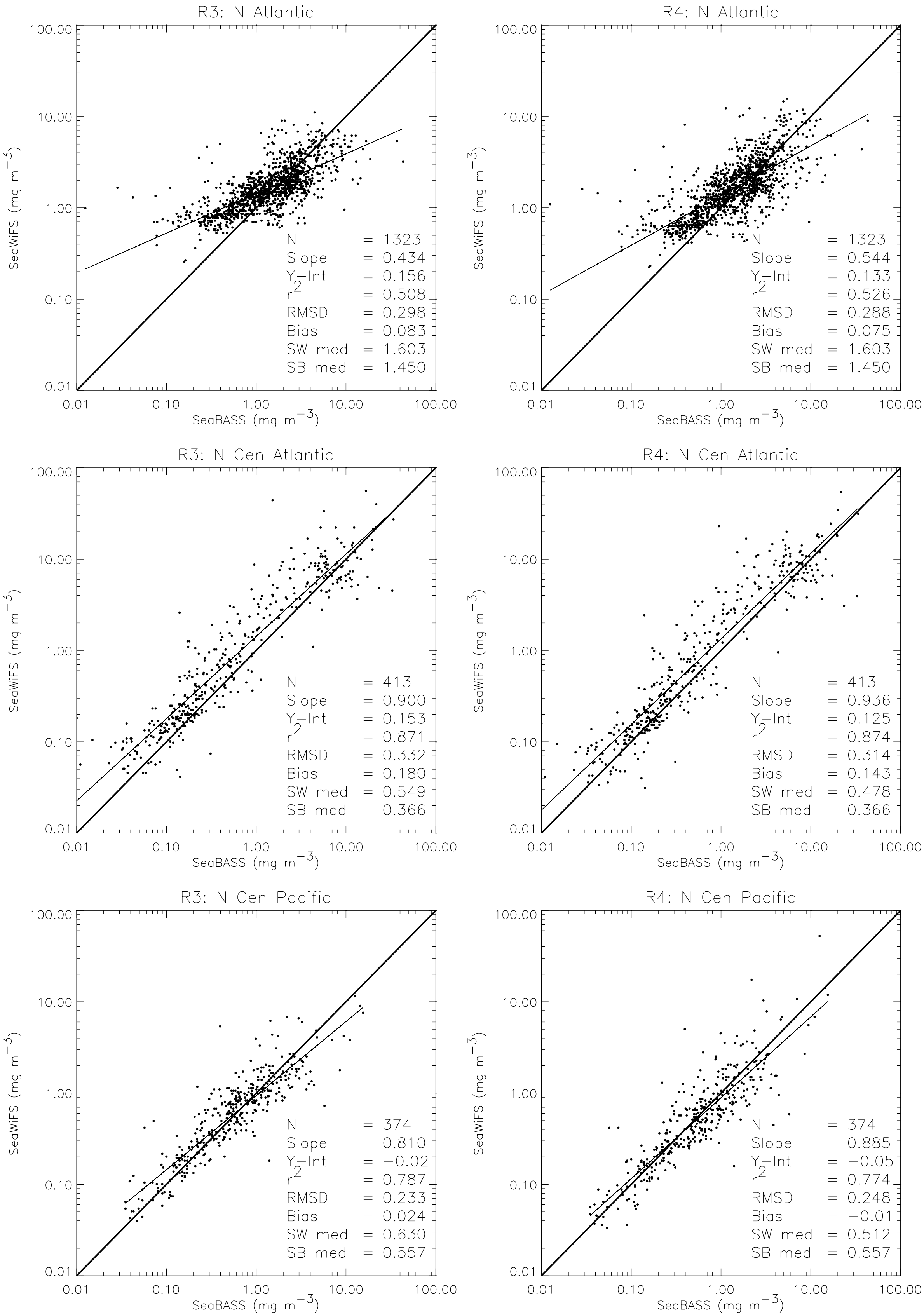
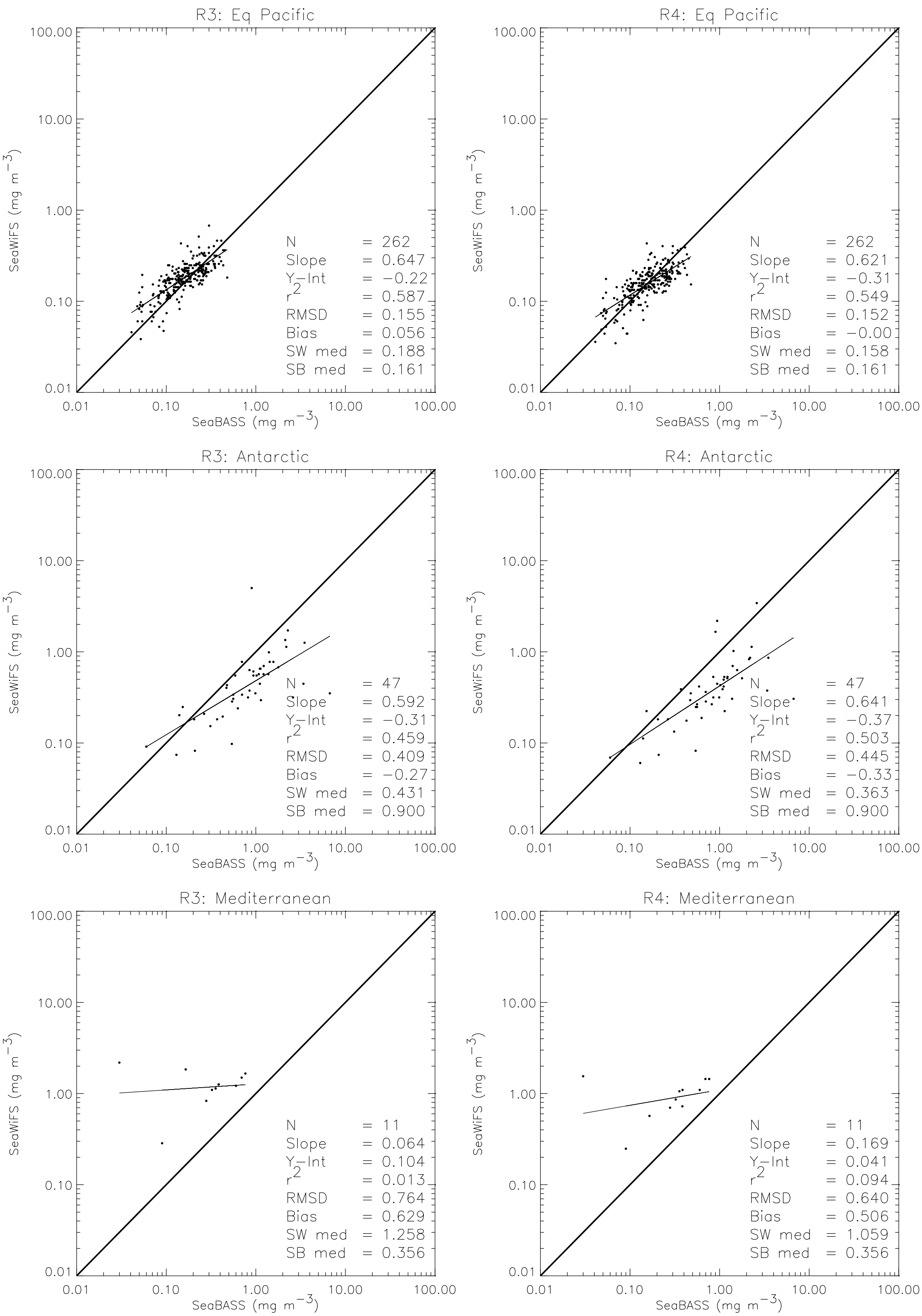


Fig. 6. Scatterplots of R3 (left) and R4 (right) SeaWiFS versus SeaBASS for six regions. Linear regression coefficients are shown, and the medians for SeaWiFS ('SW med') and SeaBASS ('SB med') are in mg m^{-3} .


R3: Eq Pacific
N = 262
Slope = 0.647
Y-Int = −0.22
r2 = 0.587
RMSD = 0.155
Bias = 0.056
SW med = 0.188
SB med = 0.161
R4: Eq Pacific
N = 262
Slope = 0.621
Y-Int = −0.31
r2 = 0.549
RMSD = 0.152
Bias = −0.00
SW med = 0.158
SB med = 0.161
R3: Antarctic
N = 47
Slope = 0.592
Y-Int = −0.31
r2 = 0.459
RMSD = 0.409
Bias = −0.27
SW med = 0.431
SB med = 0.900
R4: Antarctic
N = 47
Slope = 0.641
Y-Int = −0.37
r2 = 0.503
RMSD = 0.445
Bias = −0.33
SW med = 0.363
SB med = 0.900
R3: Mediterranean
N = 11
Slope = 0.064
Y-Int = 0.104
r2 = 0.013
RMSD = 0.764
Bias = 0.629
SW med = 1.258
SB med = 0.356
R4: Mediterranean
N = 11
Slope = 0.169
Y-Int = 0.041
r2 = 0.094
RMSD = 0.640
Bias = 0.506
SW med = 1.059
SB med = 0.356
SeaWiFS (mg m−3)
SeaBASS (mg m−3)
0.01
0.10
1.00
10.00
100.00

For every region, the R4 linear fit coefficients are improved over R3 except for the Equatorial Pacific but this region should not be considered problematic as its tight fit to the 1-to-1 line is reflected in its low RMSD and bias values. Indeed, for most regions, the R4 match-ups are reasonably aligned to the 1-to-1 line and the relationships are improved over R3. However, a few regions, particularly the North Atlantic, have regression coefficients that continue to stray from the 1-to-1 line. The lower chlorophyll values were overestimated by SeaWiFS in this region and the higher chlorophyll values were often underestimated, though this pattern is somewhat improved in R4 over R3. If the coastal [N=1,146] and open ocean [N=177] match-ups for the North Atlantic are compared separately, it is obvious in both cases that the low-end SeaWiFS values (less than 1 mg m^{-3}) tend to be higher than the corresponding SeaBASS measurements. However, density scatterplots showing a histogram function for this region (figure 7) reveal that many of the low chlorophyll values have decreased and so the majority of R4 match-ups are better aligned to the 1-to-1 line than R3. Therefore, the shift of low chlorophyll values having decreased in R4 from their R3 counterparts (shown in figure 4) appears to be an improvement as R4 matches up better with SeaBASS.

In almost every region, the median values for R4 are lower than R3. The R4 medians are now closer to the SeaBASS medians in all cases except for the Antarctic (figure 6). In addition, the bias for almost every region improved in R4 over R3. For R4, most regions have almost no bias or were slightly positively biased, except for the Mediterranean (N=11) and the Equatorial Atlantic (N=12) which have strong positive biases (but also very few match-up points), and the Antarctic (N=47) which has a negative bias. In fact, the Antarctic's negative bias and RMSD increased from R3 to R4, and it is clear from the scatterplot that most of the R4 values have decreased from their R3 counterparts and so the distribution has moved farther from the 1-to-1 line. This suggests that perhaps the changes made in the R4 processing that produced a general decrease in lower chlorophyll values may not work as well here, though clearly additional research is needed to draw any definitive conclusions.

3.2 Monthly Comparison of SeaWiFS Reprocessings

The global mean (non-area-weighted) of all co-located pixels (where both R3 and R4 had valid chlorophyll values) for the monthly May 1999 images slightly increased in R4 to 0.44 mg m^{-3} (+/- 1.1) from 0.42 mg m^{-3} (+/- 1.4) for R3. Yet even though the R4 mean was higher, the vast majority (almost 84%) of R4 pixels had lower values (though most were only slightly lower) than their R3 counterparts. A density scatterplot of R3 versus R4 (figure 8) depicts the trend observed earlier in which most chlorophyll values less than 1.0 mg m^{-3} have decreased from R3 to R4. Figure 9 (top) shows the frequency distribution of R4 minus R3 values. This shift is contrary to what would be expected based on the global averages but it does correspond with the decrease in median values from R3 to R4 found in the SeaBASS analysis. It is clear therefore that the global means are heavily impacted by the 13% of pixels where the R4 values were higher than R3 (about 3% had equal values for R3 and R4). In fact, there was a 64% increase in the number of chlorophyll values greater than 5 mg m^{-3} in R4 over R3, and for those R4 pixels, only 57% of the coincident R3 values were also greater than 5 mg m^{-3}. The R4 increase in high-end chlorophyll values is obvious in figure 9 (bottom) which shows the frequency of chlorophyll values between 5 and 25 mg m^{-3}.

In fact, when visually inspecting these images it appeared that there were more high-value outliers in the R4 image as compared to the R3 in the open ocean of the South Pacific, an area generally characterized by relatively homogeneous levels of low chlorophyll (figure 10). An analysis of part of this basin which included the southern edge of the SMI (between about -131.6 and -87.8

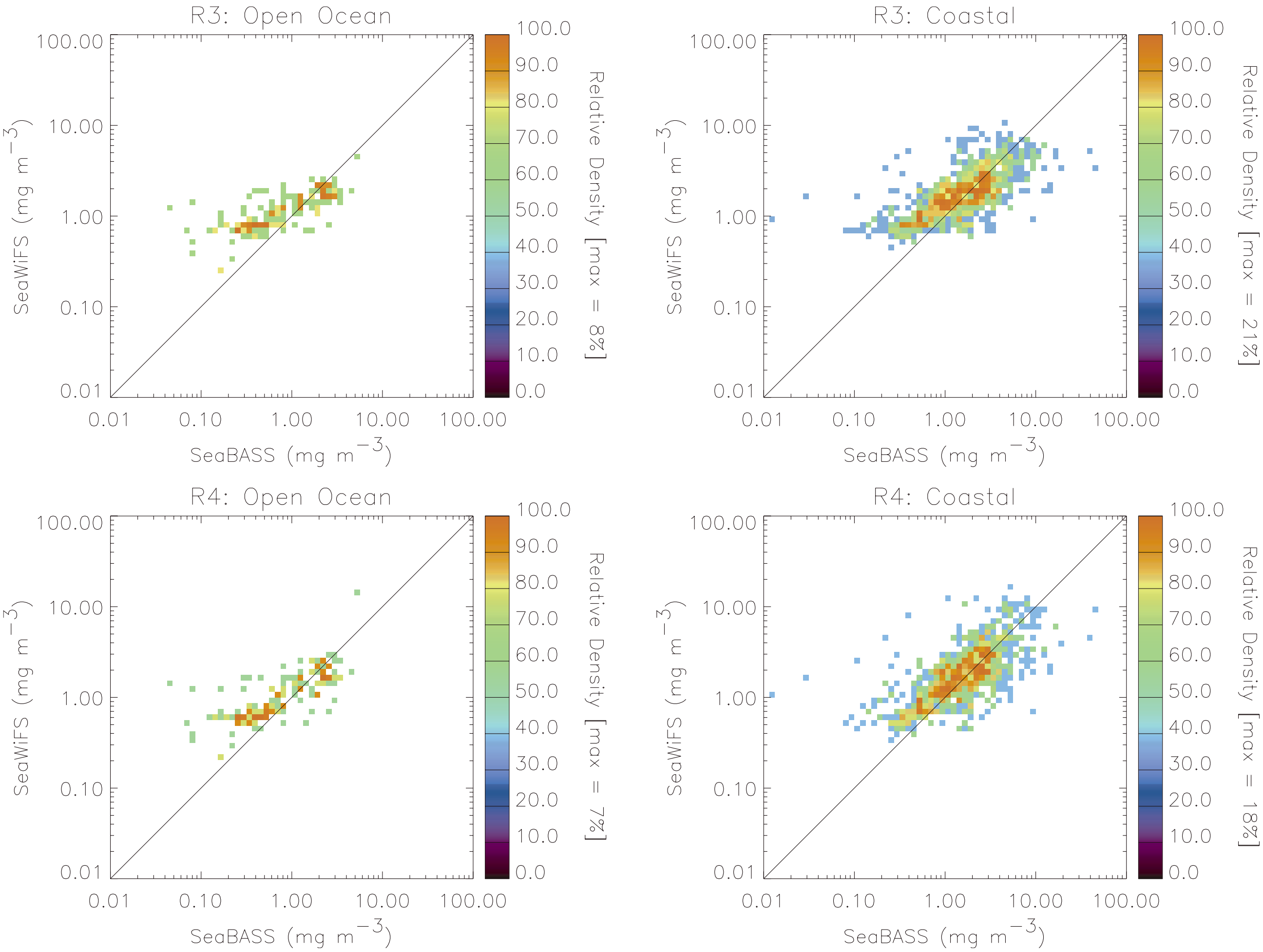


Figure 7. Scatterplots showing the relative density (histogram function) of the SeaWiFS/SeaBASS chlorophyll match-ups for the North Atlantic region. Plots on the left are SeaWiFS R3 (top) and R4 (bottom) versus SeaBASS for the open ocean (N=177); on the right are SeaWiFS R3 (top) and R4 (bottom) versus SeaBASS for the coastal areas (N=1,146). The 1-to-1 lines are shown.

degrees longitude and -59.6 and -38.6 degrees latitude) (figure 10) revealed some interesting patterns.

Chlorophyll levels have decreased overall from R3 to R4 in this area (figure 11), but a great number of high outliers are present among the ‘background’ of low chlorophyll and in many cases the relative magnitude is higher in R4 than it was in R3 (figures 11 and 12). So while there were high outliers present in the R3 data, there appears to be an increase in R4. When examining this region in detail by plotting the individual pixel values at a given longitude, high magnitude outliers well above the low-chlorophyll ‘background’ become obvious. To illustrate, we chose meridians at -120.8 and -126.9 degrees between -59.6 and -38.6 degrees latitude for R3 and R4 (figure 13). It is clear in these cases and in several other examples found that both the quantity and magnitude of high outliers have increased in this area and even some of the new R4 pixels seem to be problematic. In fact, at around 0.1 mg m^{-3} for R3 there were numerous high outliers in the R4 data (figure 14). Because the ‘back-ground’ chlorophyll is at about 0.1 mg m^{-3}, this shows a clear trend in R4 high-outlier increase when

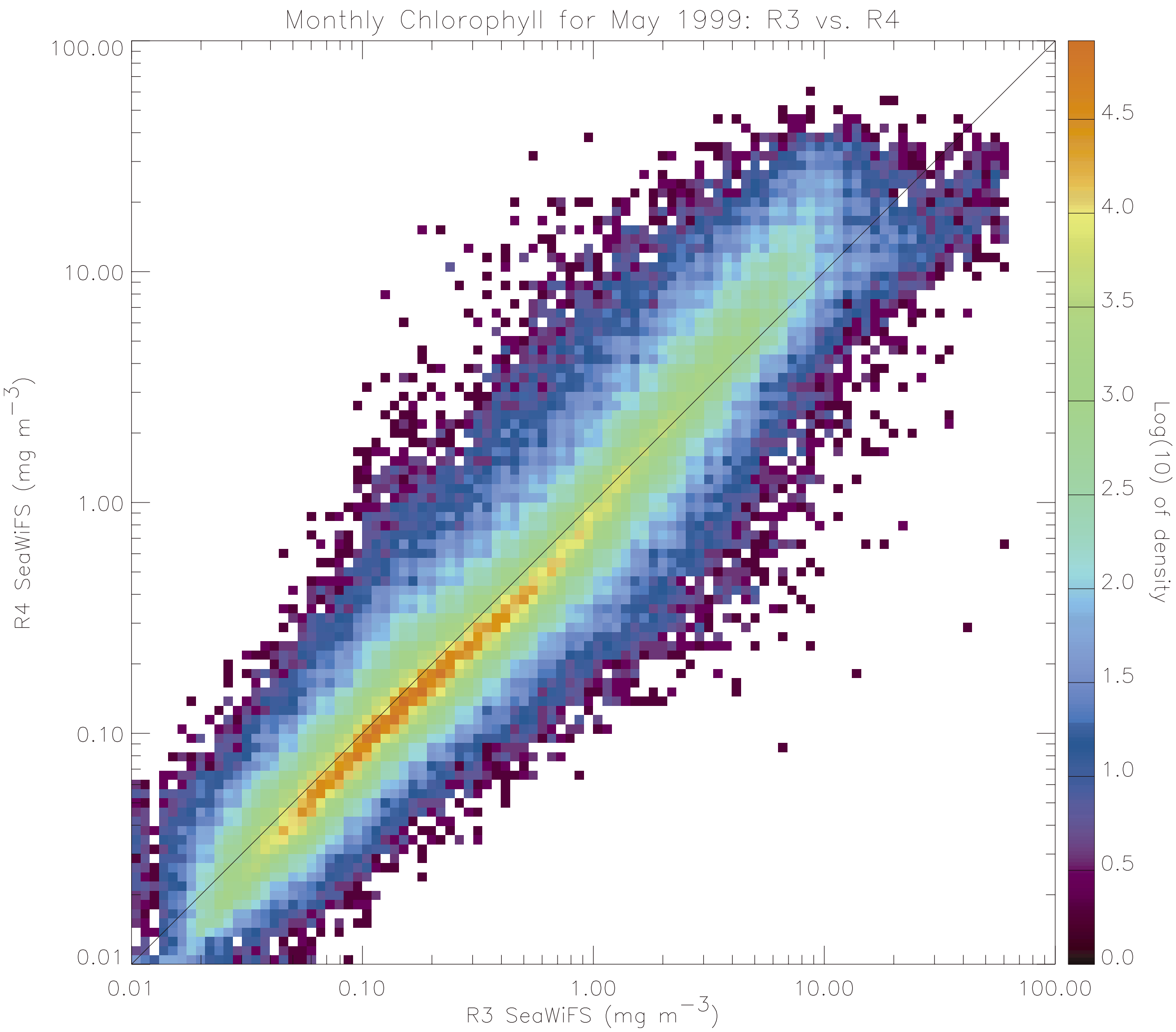


Figure 8. Scatterplot showing the relative density (histogram function) of SeaWiFS monthly chlorophyll R3 versus R4 for May 1999 (co-located points only N=3,609,956). The 1-to-1 line is shown.

they were previously in the normal range for R3. Interestingly though there is some improvement as every R3 pixel that had been a high outlier greater than 0.3 mg m^{-3} has decreased in the R4 version.

On a monthly timescale and in a largely homogenous area, increased numbers and magnitudes of high outliers in the new R4 data set as compared to the previous version is some cause for concern. The incidence of outliers should tend to be relatively low in monthly images in general due to the smoothing effects of averaging the dailies. In addition, the lower latitude areas such as the South Pacific may have fewer valid daily measurements than in other areas, but an examination of the daily images (figure 15) for this region exhibited the same general pattern shown in the monthly values.

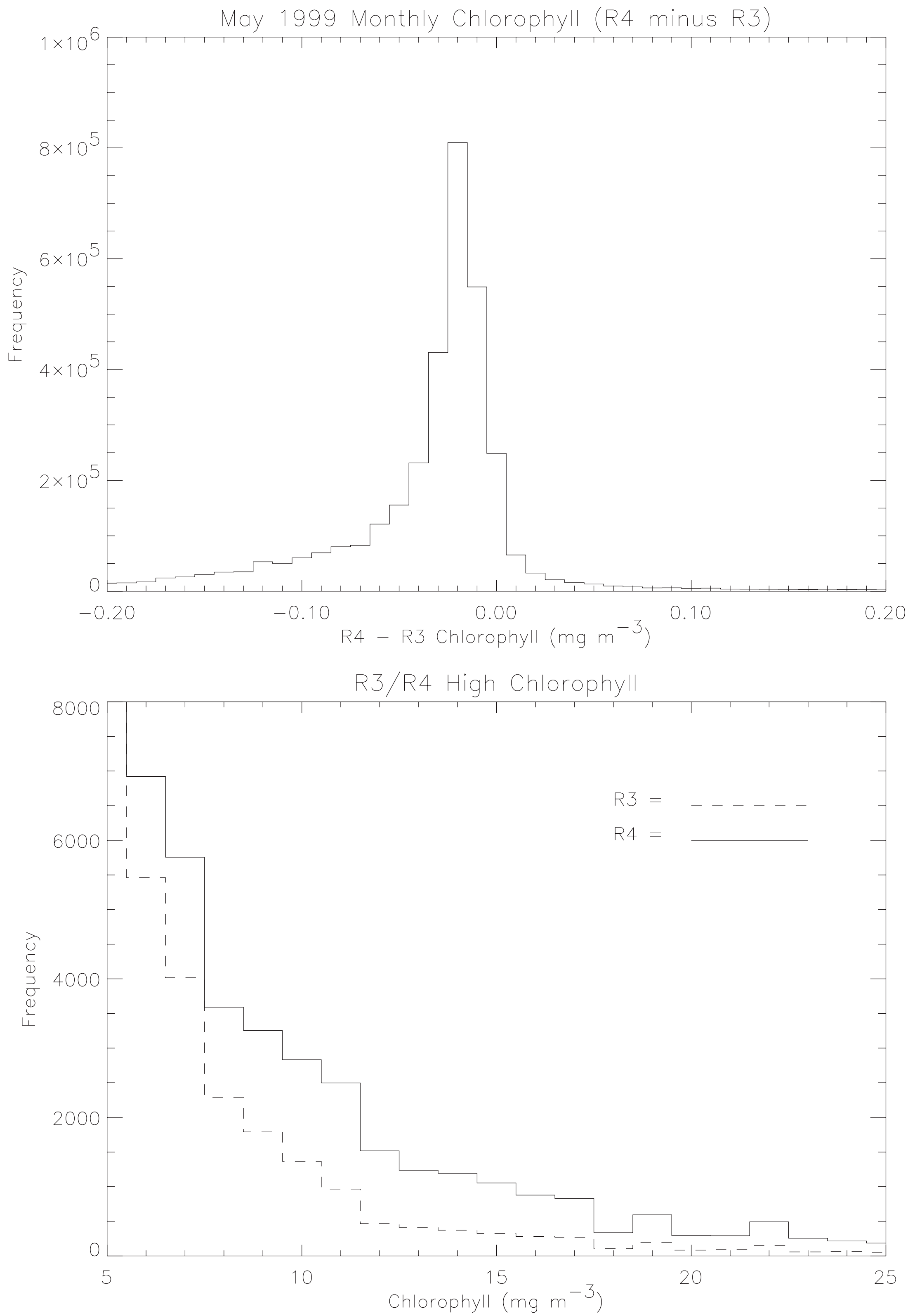


Figure 9. (Top) Histogram (binsize of 0.01) showing the frequency of values for the co-located May 1999 monthly SeaWiFS R4 SMI chlorophyll values minus the R3 counterparts (N=3,609,956). (Bottom) Histogram (binsize of 1.0) showing frequency distribution of May 1999 R3 (dashed line) and R4 (solid line) chlorophyll values between 5 and 25 mg m^{-3}.

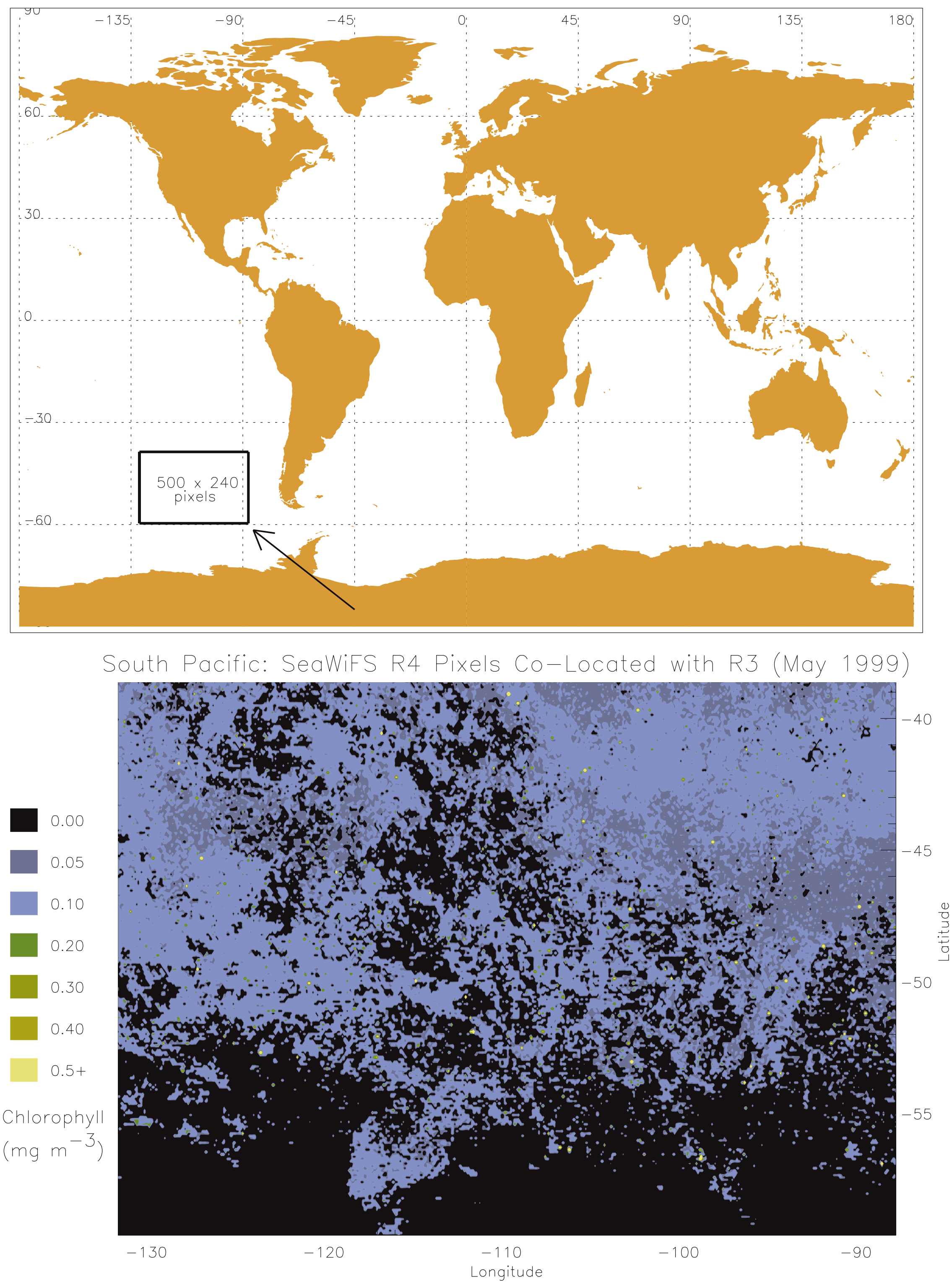


Figure 10. (Top) Global map showing the location of the South Pacific region between -131.6 and -87.8 degrees longitude and -59.6 and -38.6 degrees latitude (500 x 240 pixels). (Bottom) Contour plot of the monthly SeaWiFS R4 chlorophyll values (mg m^{-3}) which have a co-located R3 value for the South Pacific region in May 1999.

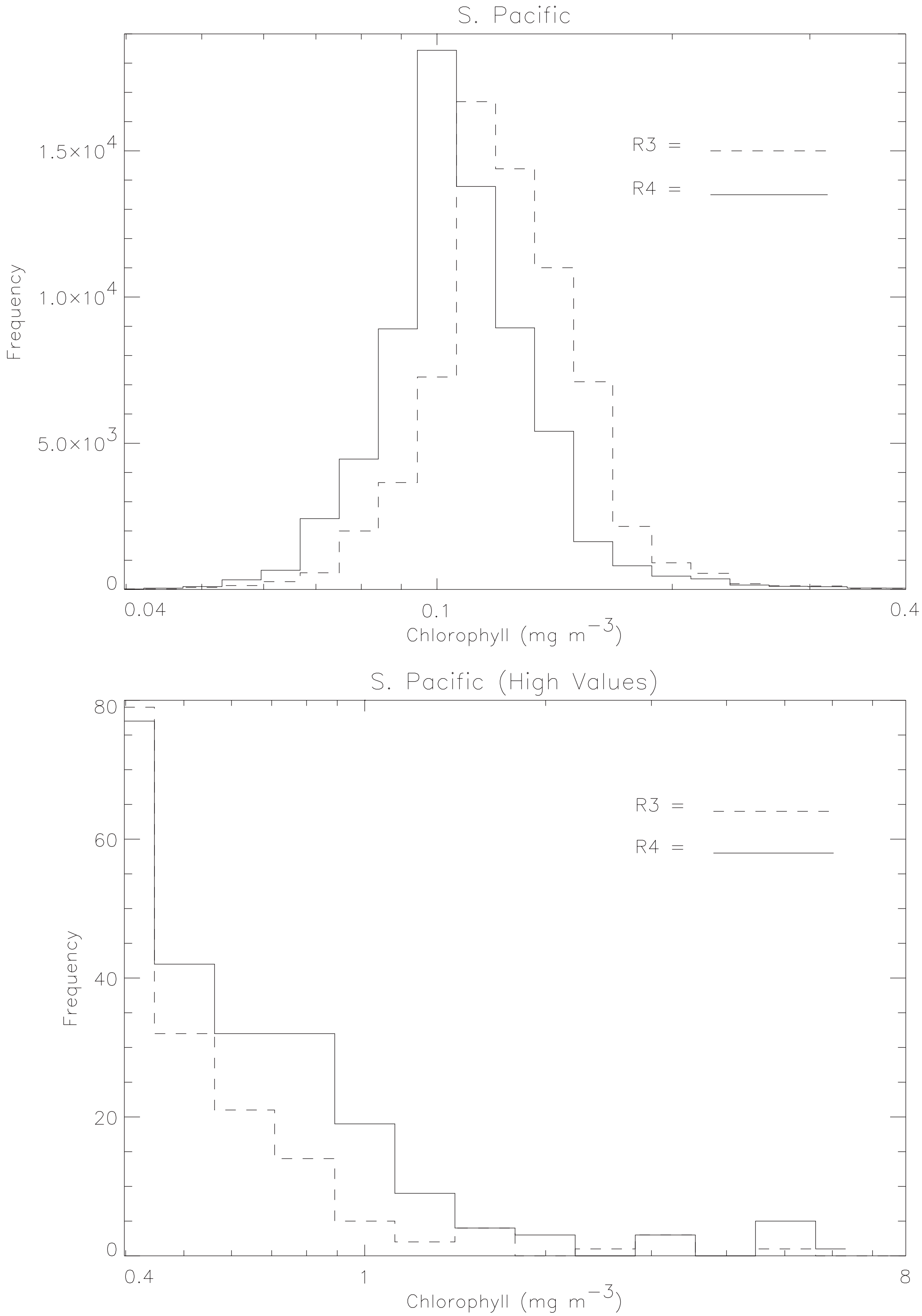


Figure 11. (Top) Histogram (binsize of 0.05) showing the frequency of log10-scaled values for SeaWiFS R3 (dashed line) and R4 (solid line) chlorophyll for the South Pacific area. (Bottom) Histogram (binsize of 0.1) showing the frequency of log10-scaled values for SeaWiFS R3 (dashed line) and R4 (solid line) chlorophyll between 0.4 and 8 mg m^{-3} for the South Pacific area.

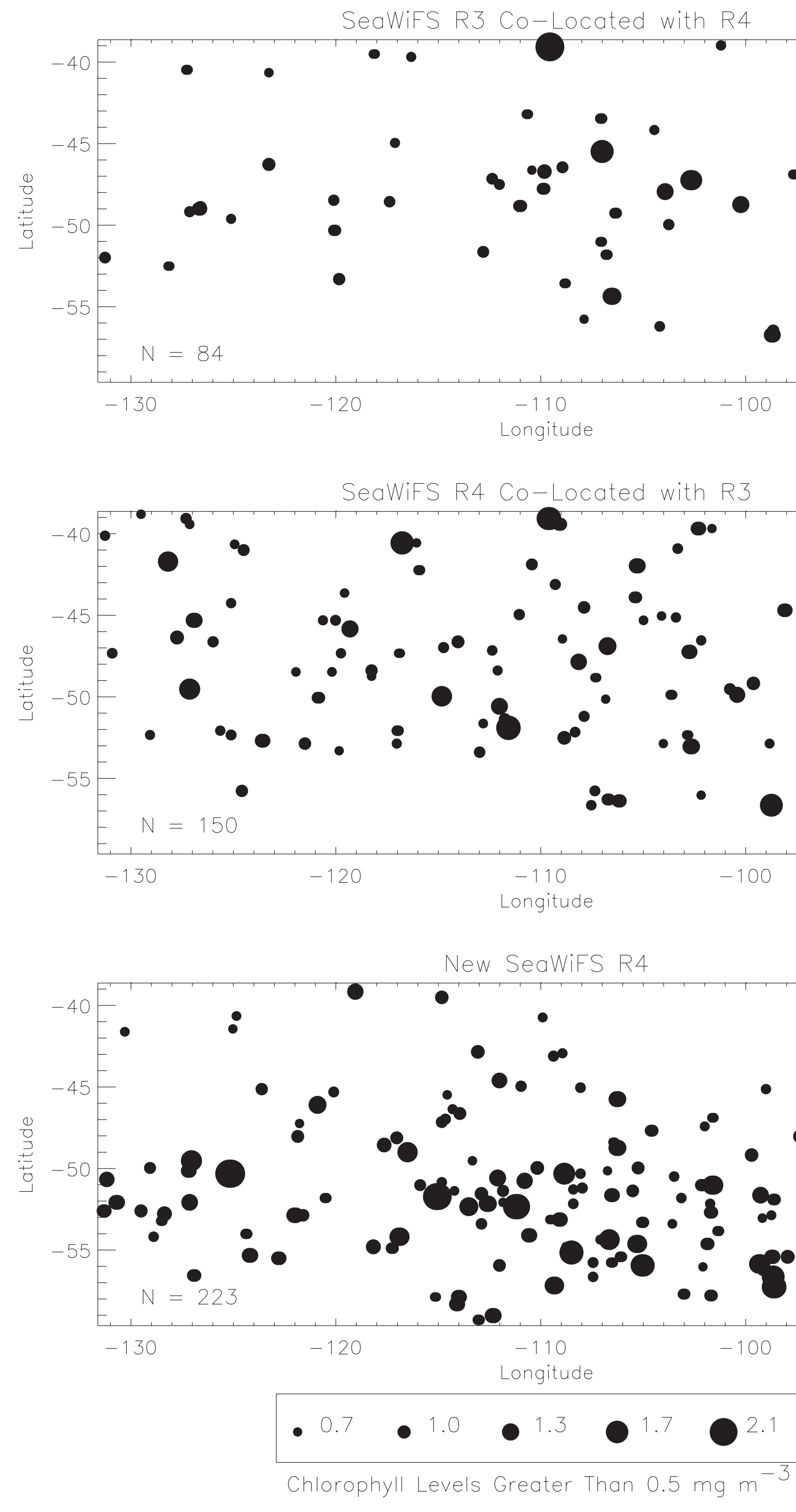


Figure 12. Plots showing the location and magnitudes of chlorophyll values greater than 0.5 mg m^{-3} in the South Pacific area for May 1999. (Top) SeaWiFS R3 with co-located R4 values [N=84]; (middle) SeaWiFS R4 with co-located R3 values [N=150]; (bottom) new SeaWiFS R4 pixels [N=223]. Representative chlorophyll values/sizes are illustrated in the box at bottom.

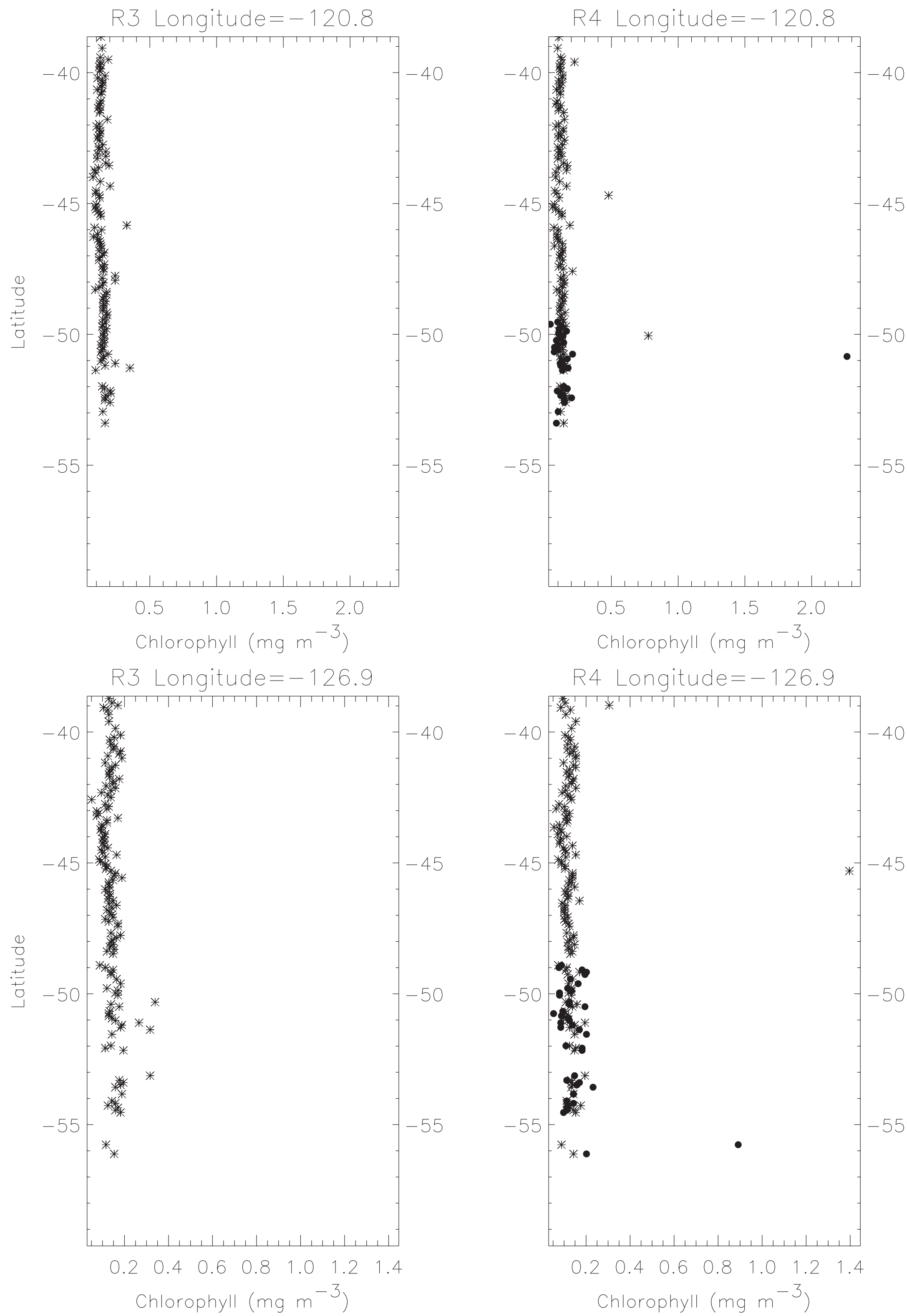


Figure 13. Chlorophyll values at meridians -120.8 degrees (top) and -126.9 degrees (bottom) between -59.6 and -38.6 degrees latitude for R3 (left) and R4 (right). Co-located (valid R3 and R4 values) are shown as asterisks and the new pixels added with the R4 processing version are shown as filled circles. The x-axis scales are data dependent.

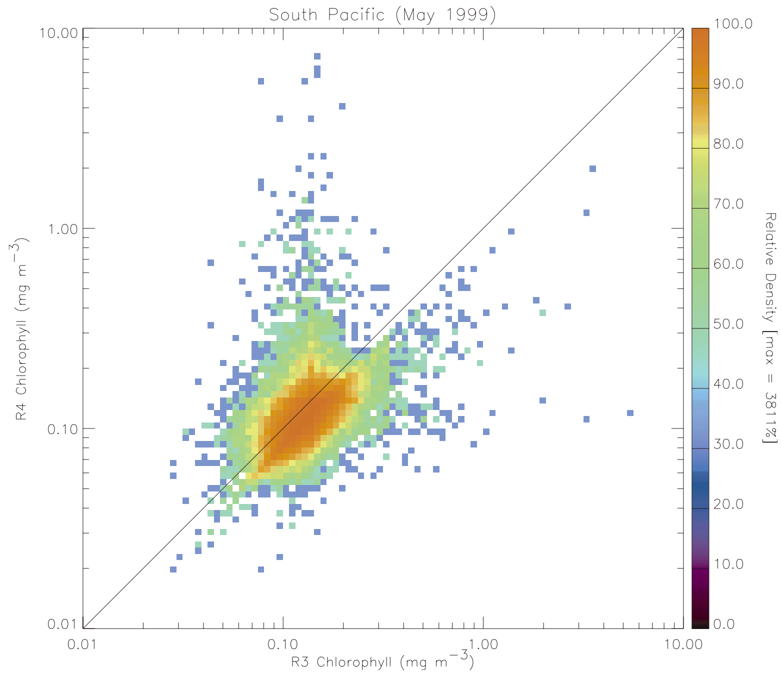


Figure 14. Scatterplot showing the relative density (histogram function) of co-located SeaWiFS R3 versus R4 monthly chlorophyll for the South Pacific region for May 1999 (N=67,443). The 1-to-1 line is shown.

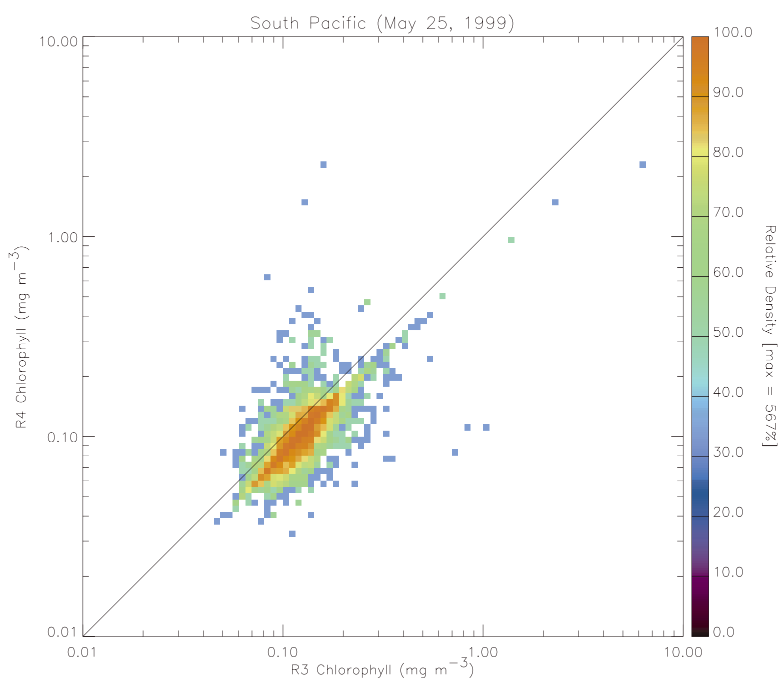


Figure 15. Scatterplot showing the relative density (histogram function) of co-located SeaWiFS R3 versus R4 daily chlorophyll for the South Pacific region for May 25, 1999 (N=9,498). The 1-to-1 line is shown.

4. CONCLUSIONS

The R4 SeaWiFS SMI chlorophyll values generally match up better with the SeaBASS in situ measurements than the R3 data set. Improvement can be seen in almost every oceanic region, except the Antarctic. However, while the match-ups improve, SeaWiFS continues to have some trouble in coastal areas, such as the North Atlantic (particularly off the coast of New England). A significant trend which improved the in situ match-ups was the overall decrease in chlorophyll levels less than 1.0 mg m^{-3}.

An examination of monthly images for May 1999 revealed that the number of high-value chlorophyll pixels had increased with R4 over R3. While outliers were present in monthly R3 SeaWiFS mapped images, it is clear that the incidence and magnitude of high outliers has increased with the R4 reprocessing in the high-latitude open ocean of the South Pacific.

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ACRONYMS

DAAC—Distributed Active Archive Center
GES—Goddard Earth Sciences
RMSD—Root Mean Squared Difference
SeaBASS—SeaWiFS Bio-Optical Archive and Storage System
SeaWiFS—Sea-Viewing Wide Field-of-View Sensor
SMI—Standard Mapped Images

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13. ABSTRACT *(Maximum 200 words)*

Satellite observations of global ocean chlorophyll from SeaWiFS were recently reprocessed to incorporate calibration and algorithm improvements. Here, comparisons are made between the newly reprocessed SeaWiFS Level-3 chlorophyll product and the previous version using in situ measurements. The results show that the newly reprocessed SeaWiFS data matches up better with the surface measurements than the previous version did. Globally, the slope of the match-ups improves to 0.85 from 0.78 in log-log scale. A significant trend that contributed to this improvement was the overall decrease in SeaWiFS chlorophyll levels less than 1.0 mg m^{-3}. Regional analyses reveal that the match-ups improve in every oceanic basin, except the Antarctic. However, SeaWiFS continues to exhibit poor correspondence with in situ data in the North Atlantic where the match-ups have a slope of 0.54. Also, an examination of monthly images for May 1999 revealed that the number and magnitude of high-value chlorophyll pixels had increased in the high-latitude open ocean of the South Pacific.

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